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L SHELL XANES FOR SOLID METALS:
Ti, V, Cr, Fe, Ni, Cu

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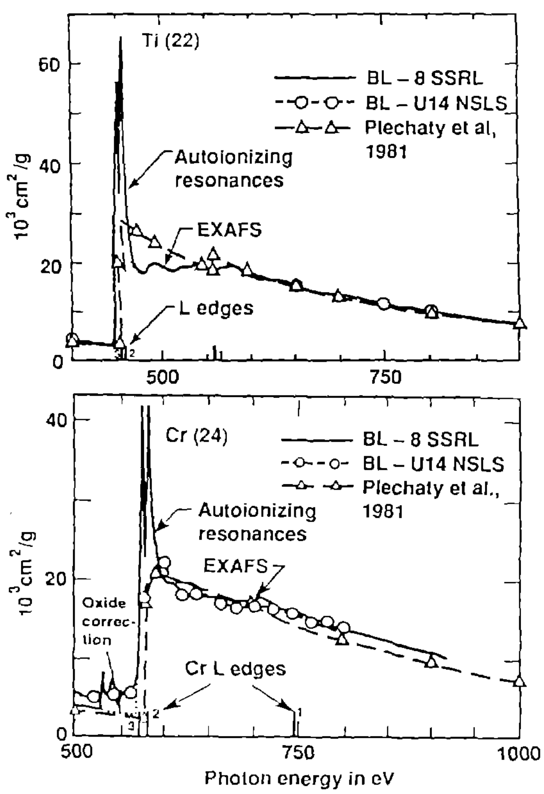
Introduction

The *L* shell x-ray absorption near edge structure (XANES) for the 3*d* transition metals Ca-Cu is dominated by atomic-like behavior which is poorly understood.[1] It has been studied by electron energy loss spectroscopy (EELS) and bremsstrahlung isochromat spectra (BIS).[2,3] More and better photoabsorption cross-section measurements are needed over the sparsely studied 400-1500 eV region to test theoretical methodologies which fuse atomic and condensed matter theories. Progress has been made reporting absolute photoabsorption cross sections taken with the spherical grating monochromator on beamline 8-2 at SSRL in 1989. These data were used in conjunction with data taken on beamline 3-4 at SSRL and beamline U14A at NSLS.[4-7]

Experiment

Transmission data for well characterized carbon-only and carbon-metal multilayer targets (100-4000 nm thick) were recorded with a resolution of 1 eV or better for Ti, V, Cr, Fe, Ni and Cu. Absolute cross sections in Figure 1 had overall uncertainties of 10% or less. Comparisons are made with previous results.[8,9] Away from edges, targets had photon penetration depths 1/3 to 3 mean free paths thick. Thinner targets (by a factor of 3 or 4) were used to resolve XANES shown in Figure 2.



Corrections for oxide impurities were possible since synchrotron radiation sources allowed continuous coverage across the oxygen K absorption edge at 543 eV. The determination of the target metallic areal densities (mass per unit area) was known to better than ± 10%. Targets were characterized for their total as well as component element purity, weight-per-unit area, thickness and composition, using very accurate balances, ion back-scattering, and particle-induced x-ray emission.

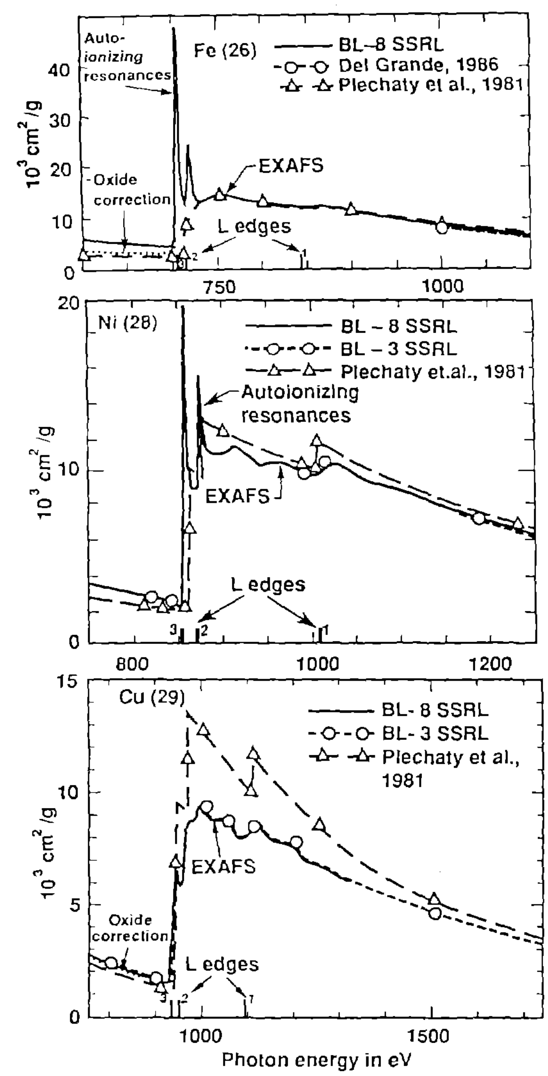


Figure 1. Photoabsorption cross section measurements in cm^2/g with 10% overall uncertainties are compared with the 1981 LLNL sub-keV theoretical data base[8] and other data[9] for five 3*d* solid metals: Ti, Cr, Fe, Ni, Cu. See reference [7].

Discussion

The Figure 1 comparisons of experiment with single particle Hartree Slater (HS) theory[8] shown as a long dashed line agree for most $3d$ metals below and at twice the energy of the ionization threshold. The $2p$-$3d$ autoionizing resonances of Figure 2 are associated with bound-bound transitions which lead to non-radiative Auger decay. What is measured is a combination of the bound-bound photoabsorption and bound-free photoionization cross sections. The HS calculation [in 8] does not include the bound-bound component for the atom or band theory to address the behavior of the solid.

There is good qualitative agreement between L shell XANES and calculations which use a multi-configuration Dirac Fock (MCDF) model with the assumption of a statistical distribution for the initial atomic states.

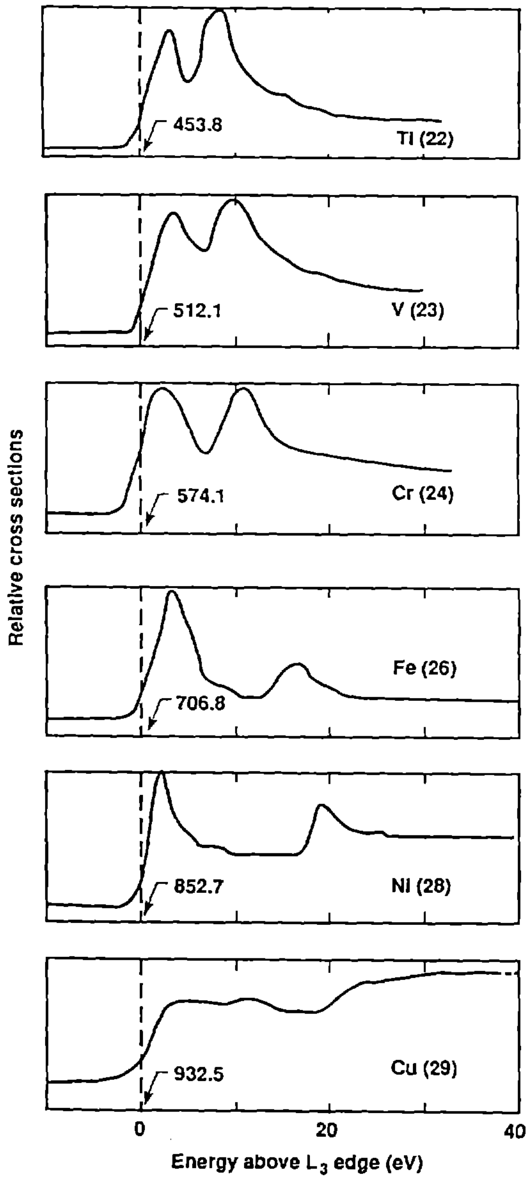


Figure 2. Measured XANES for the transition metals Ti, V, Cr, Fe, Ni and Cu showing the atomic-like $2p$-$3d$ autoionizing resonances which dominate the L_3 and L_2 edge structure.[7]

Calculations were performed in intermediate coupling with configuration interactions.[7] It is not yet clear why the statistical distribution rather than the ground state distribution for the initial states produces the measured XANES for solid metals shown in Figure 3.

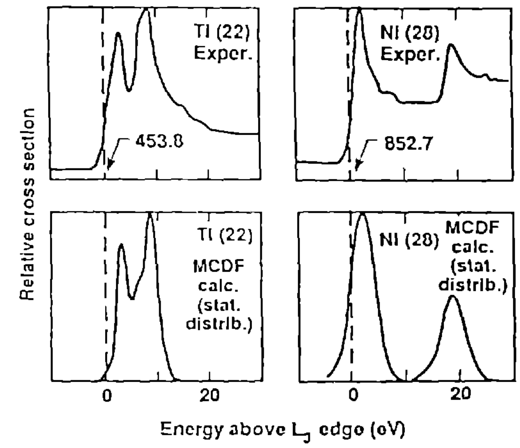


Figure 3. A comparison of measurement with calculation for L shell autoionizing resonances of solid metals dominated by atomic-like behavior. (Calculation by Mau H. Chen.)

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